Supplementary Information for:

Bioinorganic chemistry of Parkinson disease: Affinity and structural features of Cu(I) binding to the full-length β-Synuclein protein

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Calculation of the conditional dissociation constants ($^{c}K_d$) values

The correction of the apparent K_d ($^{a}K_d$) values calculated from the NMR experiments to obtain the conditional K_d ($^{c}K_d$) values was performed as reported for Cu(II) complexes.[1,2] The main components of the buffer that could act as Cu(I) binding competitors are MES buffer and Cl^- ions. Cu(I) coordination by MES has not been reported; however, MOPS and HEPES, which have similar chemical structures, are usually used in Cu(I) constant binding determinations and are considered to have practically no affinity for Cu(I).[3–5] Thus, MES competition for Cu(I) may be considered negligible in the presence of 100 mM Cl^-. The equation used to calculate the $^{c}K_d$ was:

$$^{c}K_d = \frac{^{a}K_d}{\left(1 + \beta_2.[Cl^-]^2 + \beta_3.[Cl^-]^3\right)}$$

Since Cl^- ions are in large excess (100 mM) as compared to Cu(I) (100 μM), the $[Cl^-]$ in the equation was considered to be the total $[Cl^-]_o$. The major Cu(I)-Cl^- complexes involved are $CuCl_2^-$ and $CuCl_3^{2-}$ ($\beta_2 = 3x10^5\ M^{-2}$ and $\beta_3 = 6.4x10^4\ M^{-2}$, respectively).[6]

(1) Trapaidze, A.; Hureau, C.; Bal, W.; Winterhalter, M.; Faller, P. Thermodynamic study of Cu2+ binding to the DAHK and GHK peptides by isothermal titration calorimetry (ITC) with the weaker competitor glycine. *J. Biol. Inorg. Chem.* **2012**, *17*, 37–47.

(2) Zawisza, I.; Rózga, M.; Bal, W. Affinity of copper and zinc ions to proteins and peptides related to neurodegenerative conditions (Aβ, APP, α-synuclein, PrP). *Coord. Chem. Rev.* **2017**, *256*, 2297-2307.

(3) Xiao, Z.; Brose, J.; Schimo, S.; Ackland, S. M.; La Fontaine, S.; Wedd, A. G. Unification of the copper(I) binding affinities of the metallo-chaperones Atx1, Atox1, and related proteins: detection probes and affinity standards. *J. Biol. Chem.* **2011**, *286*, 11047–11055.

(4) Bagchi, P.; Morgan, M. T.; Bacsa, J.; Fahrni, C. J. Robust affinity standards for Cu(I) biochemistry. *J. Am. Chem. Soc.* **2013**, *135*, 18549–18559.

(5) Johnson, D. K.; Stevenson, M. J.; Almadidy, Z. A.; Jenkins, S. E.; Wilcox, D. E.; Grossoehme, N. E. Stabilization of Cu(I) for binding and calorimetric measurements in aqueous solution. *Dalton Trans.* **2015**, *44*, 16494–16505.

(6) Fritz, J. J. Chloride complexes of copper(I) chloride in aqueous solution. *J. Phys. Chem.* **1980**, *84*, 2241–2246.

Figure S1

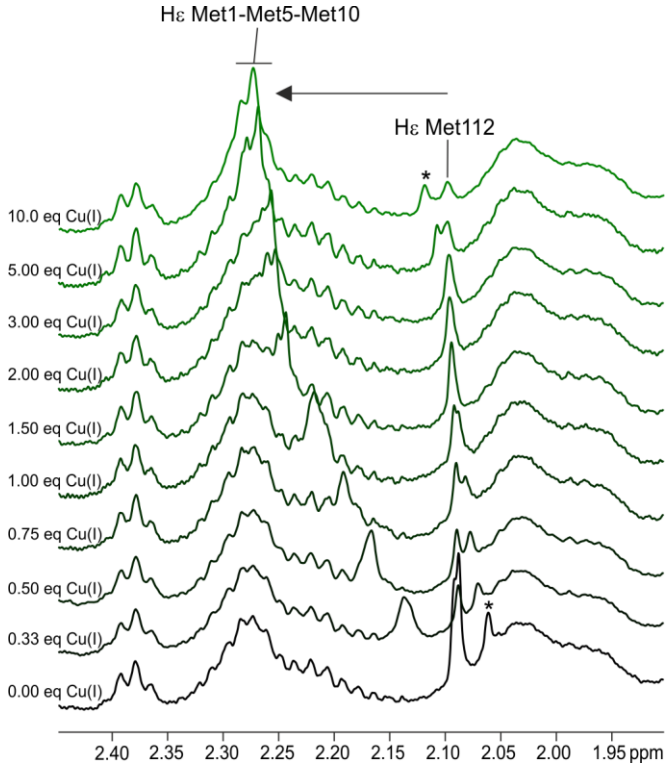

Figure S1. Cu(I) binding to site 1 of the full-length AcβS protein. 1D ^{1}H NMR spectra (1.90−2.45 ppm) of full-length AcβS in the presence of increasing Cu(I) concentrations. From black to green: 0, 0.25, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 5.0 and 10.0 equivalents of Cu(I). Changes in the chemical shifts (Δδ) corresponding to the Hε protons in the S−CH_3 groups of Met-1, Met-5, Met-10 and Met-112 residues are identified. The signal corresponding to the proton resonances in the acetyl group of Met-1 is identified with an asterisk (*). Experiments were performed using non-labeled and ^{15}N isotopically enriched AcβS samples (20 μM) in buffer A at 15 °C.

Figure S2

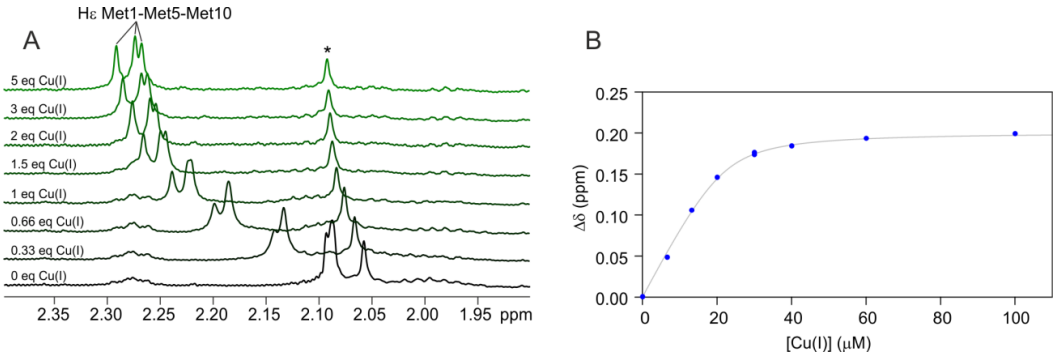

Figure S2. Affinity features of Cu(I) binding to the 1-15 AcβS peptide. **(A)** 1D ^{1}H NMR spectra (1.90−2.40 ppm) of the 1-15 AcβS peptide in the presence of increasing Cu(I) concentrations. From black to green: 0, 0.3, 0.7, 1.0, 1.5, 2.0, 3.0 and 5.0 equivalents of Cu(I). Changes in the chemical shifts (Δδ) corresponding to the Hε protons in the S−CH_3 groups of the Met-1, Met-5 and Met-10 residues are identified. The signal corresponding to the proton resonances in the acetyl group of Met-1 is identified with an asterisk (*). **(B)** Average binding curves of Cu(I) to 1-15 AcβS peptide, as monitored by changes in chemical shift of Hε signals of Met-1, Met-5 and Met-10 residues. The curve represents the fit to the model described in the text, using the program DynaFit. Experiments were performed using 1-15 AcβS peptide samples (20 μM) in buffer A at 15 °C.

Figure S3

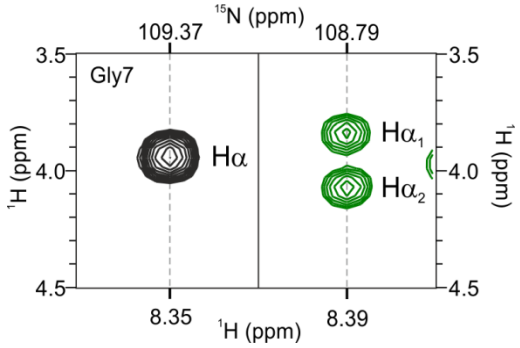

Figure S3. HN-Hα strips of the HNHA experiment corresponding to Gly-7 resonance in AcβS (black) and AcβS-Cu(I) (green). Experiments were recorded at 15^{o}C using ^{15}N AcβS (200 μM) samples dissolved in buffer A in the absence and presence of 2 equivalents of Cu(I).

Table S1. Chemical Shift Table of AcβS, in buffer MES 20mM, NaCl 100mM, pH 6.5, 288K.

Residue number	Residue ID	Atom ID	Chemical shift
1	MET	C	176.580
1	MET	CA	55.963
1	MET	CB	32.817
1	MET	H	8.453
1	MET	HA	4.429
1	MET	N	125.852
2	ASP	C	176.655
2	ASP	CA	54.467
2	ASP	CB	40.699
2	ASP	H	8.531
2	ASP	HA	4.567
2	ASP	N	120.910
3	VAL	C	176.519
3	VAL	CA	63.246
3	VAL	CB	32.318
3	VAL	H	7.909
3	VAL	HA	3.960
3	VAL	N	119.431
4	PHE	C	176.338
4	PHE	CA	58.358
4	PHE	CB	39.103
4	PHE	H	8.207
4	PHE	HA	4.567
4	PHE	N	122.602
5	MET	C	176.444
5	MET	CA	55.863
5	MET	CB	32.318
5	MET	H	8.233
5	MET	HA	4.354
5	MET	N	121.064
6	LYS	C	177.366
6	LYS	CA	57.160
6	LYS	CB	32.518
6	LYS	H	8.219
6	LYS	HA	4.198
6	LYS	N	121.939
7	GLY	C	174.433
7	GLY	CA	45.388
7	GLY	H	8.347
7	GLY	HA2	3.942
7	GLY	HA3	3.942
7	GLY	N	109.381
8	LEU	C	177.759
8	LEU	CA	55.365
8	LEU	CB	42.295
8	LEU	H	8.009
8	LEU	HA	4.354
8	LEU	N	121.526
9	SER	C	174.720
9	SER	CA	58.457
9	SER	CB	63.545
9	SER	H	8.312
9	SER	HA	4.417
9	SER	N	116.189
10	MET	C	176.081
10	MET	CA	55.464
10	MET	CB	32.718
10	MET	H	8.350
10	MET	N	122.296
11	ALA	C	177.834
11	ALA	CA	52.571
11	ALA	CB	19.049
11	ALA	H	8.252
11	ALA	HA	4.304
11	ALA	N	125.100
12	LYS	C	176.716
12	LYS	CA	56.362
12	LYS	CB	32.917
12	LYS	H	8.343
12	LYS	HA	4.286
12	LYS	N	120.951
13	GLU	C	177.060
13	GLU	CA	56.661
13	GLU	CB	30.024
13	GLU	H	8.485
13	GLU	HA	4.254
13	GLU	N	121.826
14	GLY	C	174.040
14	GLY	CA	45.188
14	GLY	H	8.454
14	GLY	HA2	3.948
14	GLY	HA3	3.948
14	GLY	N	110.083
15	VAL	C	176.474
15	VAL	CA	62.647
15	VAL	CB	32.418
15	VAL	H	7.985
15	VAL	HA	4.098
15	VAL	N	120.153
16	VAL	C	176.020
16	VAL	CA	62.448
16	VAL	CB	32.518

Residue number	Residue ID	Atom ID	Chemical shift
16	VAL	H	8.303
16	VAL	HA	4.067
16	VAL	N	125.128
17	ALA	C	177.668
17	ALA	CA	52.471
17	ALA	CB	18.950
17	ALA	H	8.463
17	ALA	HA	4.286
17	ALA	N	128.362
18	ALA	C	177.925
18	ALA	CA	52.571
18	ALA	CB	18.950
18	ALA	H	8.328
18	ALA	HA	4.236
18	ALA	N	123.681
19	ALA	C	178.182
19	ALA	CA	52.671
19	ALA	CB	19.049
19	ALA	H	8.292
19	ALA	HA	4.267
19	ALA	N	123.120
20	GLU	C	176.852
20	GLU	CA	56.661
20	GLU	CB	30.124
20	GLU	H	8.354
20	GLU	HA	4.229
20	GLU	N	120.099
21	LYS	C	177.109
21	LYS	CA	56.562
21	LYS	CB	32.718
21	LYS	H	8.359
21	LYS	N	122.281
22	THR	C	174.690
22	THR	CA	62.248
22	THR	CB	69.731
22	THR	H	8.150
22	THR	HA	4.279
22	THR	N	115.224
23	LYS	C	176.595
23	LYS	CA	56.661
23	LYS	CB	32.718
23	LYS	H	8.358
23	LYS	HA	4.292
23	LYS	N	123.834
24	GLN	C	177.018
24	GLN	CA	56.262

Residue number	Residue ID	Atom ID	Chemical shift
24	GLN	CB	29.325
24	GLN	H	8.440
24	GLN	HA	4.267
24	GLN	N	121.779
25	GLY	C	174.161
25	GLY	CA	45.288
25	GLY	H	8.512
25	GLY	HA2	3.973
25	GLY	HA3	3.973
25	GLY	N	110.552
26	VAL	C	176.731
26	VAL	CA	62.548
26	VAL	CB	32.518
26	VAL	H	8.094
26	VAL	HA	4.173
26	VAL	N	119.670
27	THR	C	174.645
27	THR	CA	62.149
27	THR	CB	69.631
27	THR	H	8.337
27	THR	HA	4.342
27	THR	N	118.571
28	GLU	C	176.338
28	GLU	CA	56.462
28	GLU	CB	30.124
28	GLU	H	8.522
28	GLU	HA	4.267
28	GLU	N	124.082
29	ALA	C	177.759
29	ALA	CA	52.671
29	ALA	CB	18.950
29	ALA	H	8.393
29	ALA	HA	4.254
29	ALA	N	125.205
30	ALA	C	178.167
30	ALA	CA	52.671
30	ALA	CB	19.049
30	ALA	H	8.279
30	ALA	HA	4.273
30	ALA	N	123.299
31	GLU	C	176.791
31	GLU	CA	56.661
31	GLU	CB	30.124
31	GLU	H	8.368
31	GLU	HA	4.229
31	GLU	N	119.930

Residue number	Residue ID	Atom ID	Chemical shift
32	LYS	C	177.063
32	LYS	CA	56.562
32	LYS	CB	32.917
32	LYS	H	8.340
32	LYS	HA	4.361
32	LYS	N	122.215
33	THR	C	174.766
33	THR	CA	62.049
33	THR	CB	69.731
33	THR	H	8.185
33	THR	HA	4.304
33	THR	N	115.407
34	LYS	C	176.610
34	LYS	CA	56.562
34	LYS	CB	32.718
34	LYS	H	8.407
34	LYS	HA	4.279
34	LYS	N	123.704
35	GLU	C	177.018
35	GLU	CA	56.661
35	GLU	CB	29.924
35	GLU	H	8.423
35	GLU	HA	4.261
35	GLU	N	121.697
36	GLY	C	174.055
36	GLY	CA	45.288
36	GLY	H	8.447
36	GLY	HA2	3.954
36	GLY	HA3	3.954
36	GLY	N	109.938
37	VAL	C	175.960
37	VAL	CA	62.348
37	VAL	CB	32.518
37	VAL	H	7.924
37	VAL	HA	4.054
37	VAL	N	119.571
38	LEU	C	176.701
38	LEU	CA	54.866
38	LEU	CB	42.295
38	LEU	H	8.290
38	LEU	HA	4.329
38	LEU	N	125.662
39	TYR	C	175.612
39	TYR	CA	57.958
39	TYR	CB	38.604
39	TYR	H	8.285

Residue number	Residue ID	Atom ID	Chemical shift
39	TYR	HA	4.586
39	TYR	N	122.355
40	VAL	C	176.202
40	VAL	CA	62.149
40	VAL	CB	32.618
40	VAL	H	8.097
40	VAL	HA	4.060
40	VAL	N	123.244
41	GLY	C	173.995
41	GLY	CA	45.188
41	GLY	H	8.081
41	GLY	HA2	3.935
41	GLY	HA3	3.935
41	GLY	N	112.172
42	SER	C	174.826
42	SER	CA	58.258
42	SER	CB	63.745
42	SER	H	8.271
42	SER	HA	4.442
42	SER	N	115.651
43	LYS	C	176.882
43	LYS	CA	56.462
43	LYS	CB	32.917
43	LYS	H	8.494
43	LYS	HA	4.423
43	LYS	N	123.418
44	THR	C	174.599
44	THR	CA	61.949
44	THR	CB	69.731
44	THR	H	8.207
44	THR	HA	4.304
44	THR	N	115.316
45	ARG	C	176.217
45	ARG	CA	56.163
45	ARG	CB	30.622
45	ARG	H	8.449
45	ARG	HA	4.323
45	ARG	N	123.405
46	GLU	C	176.942
46	GLU	CA	56.661
46	GLU	CB	30.124
46	GLU	H	8.498
46	GLU	HA	4.261
46	GLU	N	122.159
47	GLY	C	173.934
47	GLY	CA	45.188

Residue number	Residue ID	Atom ID	Chemical shift
47	GLY	H	8.487
47	GLY	HA2	3.954
47	GLY	HA3	3.954
47	GLY	N	110.080
48	VAL	C	176.308
48	VAL	CA	62.248
48	VAL	CB	32.618
48	VAL	H	7.954
48	VAL	HA	4.123
48	VAL	N	119.921
49	VAL	C	176.066
49	VAL	CA	62.248
49	VAL	CB	32.518
49	VAL	H	8.383
49	VAL	HA	4.092
49	VAL	N	125.454
50	GLN	C	176.308
50	GLN	CA	55.963
50	GLN	CB	29.425
50	GLN	H	8.601
50	GLN	HA	4.336
50	GLN	N	125.300
51	GLY	C	173.904
51	GLY	CA	45.089
51	GLY	H	8.507
51	GLY	HA2	3.960
51	GLY	HA3	3.960
51	GLY	N	110.782
52	VAL	C	176.051
52	VAL	CA	62.049
52	VAL	CB	32.718
52	VAL	H	8.069
52	VAL	HA	4.135
52	VAL	N	119.569
53	ALA	C	177.774
53	ALA	CA	52.471
53	ALA	CB	19.149
53	ALA	H	8.501
53	ALA	HA	4.348
53	ALA	N	128.063
54	SER	C	174.735
54	SER	CA	58.158
54	SER	CB	63.845
54	SER	H	8.364
54	SER	HA	4.448
54	SER	N	115.905

Residue number	Residue ID	Atom ID	Chemical shift
55	VAL	C	176.217
55	VAL	CA	62.548
55	VAL	CB	32.518
55	VAL	H	8.246
55	VAL	HA	4.104
55	VAL	N	122.055
56	ALA	C	178.061
56	ALA	CA	52.671
56	ALA	CB	19.049
56	ALA	H	8.377
56	ALA	HA	4.286
56	ALA	N	127.299
57	GLU	C	176.942
57	GLU	CA	56.362
57	GLU	CB	30.323
57	GLU	H	8.339
57	GLU	N	120.677
58	LYS	C	177.215
58	LYS	CA	56.362
58	LYS	CB	32.717
58	LYS	H	8.416
58	LYS	HA	4.329
58	LYS	N	122.518
59	THR	C	174.917
59	THR	CA	62.248
59	THR	CB	69.731
59	THR	H	8.211
59	THR	HA	4.273
59	THR	N	115.560
60	LYS	C	177.094
60	LYS	CA	56.961
60	LYS	CB	32.618
60	LYS	H	8.366
60	LYS	HA	4.267
60	LYS	N	123.506
61	GLU	C	177.003
61	GLU	CA	57.160
61	GLU	CB	29.824
61	GLU	H	8.442
61	GLU	HA	4.254
61	GLU	N	121.883
62	GLN	C	176.202
62	GLN	CA	56.262
62	GLN	CB	29.226
62	GLN	H	8.387
62	GLN	HA	4.254

Residue number	Residue ID	Atom ID	Chemical shift
62	GLN	N	121.270
63	ALA	C	178.046
63	ALA	CA	52.771
63	ALA	CB	19.049
63	ALA	H	8.353
63	ALA	HA	4.298
63	ALA	N	124.773
64	SER	C	174.569
64	SER	CA	58.557
64	SER	CB	63.645
64	SER	H	8.258
64	SER	HA	4.367
64	SER	N	114.671
65	HIS	C	174.977
65	HIS	CA	55.963
65	HIS	CB	29.625
65	HIS	H	8.354
65	HIS	N	120.701
66	LEU	C	177.910
66	LEU	CA	55.564
66	LEU	CB	41.996
66	LEU	H	8.226
66	LEU	HA	4.304
66	LEU	N	123.165
67	GLY	C	174.660
67	GLY	CA	45.288
67	GLY	H	8.443
67	GLY	HA2	3.960
67	GLY	HA3	3.960
67	GLY	N	109.733
68	GLY	C	173.828
68	GLY	CA	45.089
68	GLY	H	8.282
68	GLY	HA2	3.960
68	GLY	HA3	3.960
68	GLY	N	108.755
69	ALA	C	177.623
69	ALA	CA	52.372
69	ALA	CB	19.149
69	ALA	H	8.207
69	ALA	HA	4.304
69	ALA	N	123.883
70	VAL	C	175.930
70	VAL	CA	62.049
70	VAL	CB	32.817
70	VAL	H	8.104
70	VAL	HA	4.042
70	VAL	N	119.354
71	PHE	C	175.717
71	PHE	CA	57.759
71	PHE	CB	39.701
71	PHE	H	8.432
71	PHE	HA	4.692
71	PHE	N	124.484
72	SER	C	174.736
72	SER	CA	58.058
72	SER	CB	63.745
72	SER	H	8.353
72	SER	HA	4.386
72	SER	N	118.616
73	GLY	C	173.828
73	GLY	CA	45.188
73	GLY	H	7.888
73	GLY	HA2	3.917
73	GLY	HA3	3.917
73	GLY	N	110.694
74	ALA	C	178.318
74	ALA	CA	52.652
74	ALA	CB	19.149
74	ALA	H	8.240
74	ALA	HA	4.323
74	ALA	N	123.752
75	GLY	C	173.904
75	GLY	CA	45.188
75	GLY	H	8.459
75	GLY	HA2	3.923
75	GLY	HA3	3.923
75	GLY	N	107.846
76	ASN	C	175.295
76	ASN	CA	53.070
76	ASN	CB	38.777
76	ASN	H	8.275
76	ASN	HA	4.717
76	ASN	N	118.705
77	ILE	C	176.171
77	ILE	CA	61.450
77	ILE	CB	38.469
77	ILE	H	8.140
77	ILE	HA	4.135
77	ILE	N	121.558
78	ALA	C	177.562
78	ALA	CA	52.571

Residue number	Residue ID	Atom ID	Chemical shift
78	ALA	CB	18.950
78	ALA	H	8.395
78	ALA	HA	4.273
78	ALA	N	128.066
79	ALA	C	177.759
79	ALA	CA	52.471
79	ALA	CB	19.049
79	ALA	H	8.209
79	ALA	HA	4.273
79	ALA	N	123.338
80	ALA	C	178.152
80	ALA	CA	52.571
80	ALA	CB	19.049
80	ALA	H	8.321
80	ALA	HA	4.361
80	ALA	N	123.337
81	THR	C	175.234
81	THR	CA	61.949
81	THR	CB	69.831
81	THR	H	8.101
81	THR	HA	4.323
81	THR	N	112.492
82	GLY	C	173.874
82	GLY	CA	45.188
82	GLY	H	8.370
82	GLY	HA2	3.954
82	GLY	HA3	3.954
82	GLY	N	110.802
83	LEU	C	177.260
83	LEU	CA	55.065
83	LEU	CB	42.295
83	LEU	H	8.087
83	LEU	HA	4.361
83	LEU	N	121.720
84	VAL	C	175.854
84	VAL	CA	62.049
84	VAL	CB	32.618
84	VAL	H	8.167
84	VAL	HA	4.073
84	VAL	N	122.159
85	LYS	C	176.126
85	LYS	CA	56.163
85	LYS	CB	32.817
85	LYS	H	8.496
85	LYS	HA	4.317
85	LYS	N	126.720

Residue number	Residue ID	Atom ID	Chemical shift
86	ARG	C	176.096
86	ARG	CA	56.163
86	ARG	CB	30.822
86	ARG	H	8.512
86	ARG	N	124.257
87	GLU	C	175.869
87	GLU	CA	56.262
87	GLU	CB	30.024
87	GLU	H	8.594
87	GLU	HA	4.236
87	GLU	N	122.993
88	GLU	C	175.673
88	GLU	CA	56.414
88	GLU	CB	30.323
88	GLU	H	8.386
88	GLU	N	122.244
89	PHE	C	173.828
89	PHE	CA	55.764
89	PHE	CB	39.103
89	PHE	H	8.346
89	PHE	HA	4.911
89	PHE	N	121.450
90	PRO	C	177.184
90	PRO	CA	63.246
90	PRO	CB	32.019
91	THR	C	174.312
91	THR	CA	61.750
91	THR	CB	69.731
91	THR	H	8.317
91	THR	HA	4.336
91	THR	N	114.140
92	ASP	C	175.794
92	ASP	CA	54.267
92	ASP	CB	40.998
92	ASP	H	8.378
92	ASP	N	122.385
93	LEU	C	177.048
93	LEU	CA	54.965
93	LEU	CB	42.395
93	LEU	H	8.130
93	LEU	HA	4.336
93	LEU	N	122.512
94	LYS	C	174.599
94	LYS	CA	54.267
94	LYS	CB	32.318
94	LYS	H	8.510

Residue number	Residue ID	Atom ID	Chemical shift
94	LYS	HA	4.586
94	LYS	N	124.465
95	PRO	C	177.215
95	PRO	CA	63.346
95	PRO	CB	32.019
96	GLU	C	176.685
96	GLU	CA	56.761
96	GLU	CB	29.824
96	GLU	H	8.735
96	GLU	HA	4.217
96	GLU	N	120.555
97	GLU	C	176.368
97	GLU	CA	56.366
97	GLU	CB	30.356
97	GLU	H	8.399
97	GLU	N	122.342
98	VAL	C	175.884
98	VAL	CA	62.149
98	VAL	CB	32.618
98	VAL	H	8.169
98	VAL	HA	4.079
98	VAL	N	122.004
99	ALA	C	177.668
99	ALA	CA	52.471
99	ALA	CB	19.049
99	ALA	H	8.466
99	ALA	HA	4.298
99	ALA	N	128.439
100	GLN	C	176.066
100	GLN	CA	55.764
100	GLN	CB	29.525
100	GLN	H	8.443
100	GLN	HA	4.298
100	GLN	N	120.569
101	GLU	C	176.126
101	GLU	CA	56.262
101	GLU	CB	30.124
101	GLU	H	8.530
101	GLU	HA	4.254
101	GLU	N	122.868
102	ALA	C	177.260
102	ALA	CA	52.272
102	ALA	CB	19.249
102	ALA	H	8.438
102	ALA	HA	4.317
102	ALA	N	125.784
103	ALA	C	177.608
103	ALA	CA	52.172
103	ALA	CB	19.249
103	ALA	H	8.351
103	ALA	HA	4.317
103	ALA	N	124.217
104	GLU	C	176.292
104	GLU	CA	56.063
104	GLU	CB	30.423
104	GLU	H	8.411
104	GLU	HA	4.279
104	GLU	N	120.785
105	GLU	C	174.418
105	GLU	CB	29.924
105	GLU	H	8.497
105	GLU	N	124.097
106	PRO	C	176.519
106	PRO	CA	62.947
106	PRO	CB	32.019
107	LEU	C	177.124
107	LEU	CA	54.965
107	LEU	CB	42.096
107	LEU	H	8.407
107	LEU	HA	4.342
107	LEU	N	123.224
108	ILE	C	175.914
108	ILE	CA	60.453
108	ILE	CB	38.504
108	ILE	H	8.269
108	ILE	HA	4.179
108	ILE	N	123.708
109	GLU	C	174.221
109	GLU	CA	54.267
109	GLU	CB	29.725
109	GLU	H	8.505
109	GLU	HA	4.580
109	GLU	N	127.392
110	PRO	C	176.625
110	PRO	CA	62.947
110	PRO	CB	32.019
111	LEU	C	177.290
111	LEU	CA	54.866
111	LEU	CB	42.096
111	LEU	H	8.382
111	LEU	HA	4.317
111	LEU	N	122.703

Residue number	Residue ID	Atom ID	Chemical shift
112	MET	C	175.839
112	MET	CA	54.866
112	MET	CB	32.917
112	MET	H	8.448
112	MET	HA	4.517
112	MET	N	122.455
113	GLU	C	174.418
113	GLU	CA	54.367
113	GLU	CB	29.625
113	GLU	H	8.481
113	GLU	N	124.153
114	PRO	C	177.030
114	PRO	CA	63.047
114	PRO	CB	32.019
115	GLU	C	177.079
115	GLU	CA	56.562
115	GLU	CB	30.323
115	GLU	H	8.622
115	GLU	HA	4.261
115	GLU	N	121.721
116	GLY	C	173.889
116	GLY	CA	45.089
116	GLY	H	8.456
116	GLY	HA2	3.954
116	GLY	HA3	3.954
116	GLY	N	110.239
117	GLU	C	176.338
117	GLU	CA	56.462
117	GLU	CB	30.323
117	GLU	H	8.355
117	GLU	HA	4.248
117	GLU	N	120.582
118	SER	C	173.919
118	SER	CA	57.958
118	SER	CB	63.845
118	SER	H	8.406
118	SER	HA	4.436
118	SER	N	117.088
119	TYR	C	175.355
119	TYR	CA	57.859
119	TYR	CB	38.903
119	TYR	H	8.343
119	TYR	HA	4.586
119	TYR	N	123.011
120	GLU	C	175.401
120	GLU	CA	55.764

Residue number	Residue ID	Atom ID	Chemical shift
120	GLU	CB	30.922
120	GLU	H	8.169
120	GLU	HA	4.286
120	GLU	N	123.149
121	ASP	C	173.692
121	ASP	CA	52.671
121	ASP	CB	40.200
121	ASP	H	8.447
121	ASP	HA	4.811
121	ASP	N	123.551
123	PRO	C	176.912
123	PRO	CA	62.847
123	PRO	CB	31.919
124	GLN	C	176.035
124	GLN	CA	55.664
124	GLN	CB	29.625
124	GLN	H	8.566
124	GLN	HA	4.298
124	GLN	N	121.274
125	GLU	C	176.202
125	GLU	CA	56.262
125	GLU	CB	30.223
125	GLU	H	8.556
125	GLU	HA	4.261
125	GLU	N	122.993
126	GLU	C	175.945
126	GLU	CA	56.362
126	GLU	CB	30.423
126	GLU	H	8.508
126	GLU	HA	4.254
126	GLU	N	122.456
127	TYR	C	175.316
127	TYR	CA	58.058
127	TYR	CB	38.803
127	TYR	H	8.384
127	TYR	HA	4.561
127	TYR	N	122.460
128	GLN	C	174.841
128	GLN	CA	54.965
128	GLN	CB	29.924
128	GLN	H	8.178
128	GLN	HA	4.261
128	GLN	N	123.756
129	GLU	C	175.802
129	GLU	CA	56.262
129	GLU	CB	30.223

Residue number	Residue ID	Atom ID	Chemical shift
129	GLU	H	8.381
129	GLU	HA	4.148
129	GLU	N	123.011
130	TYR	C	175.061
130	TYR	CA	57.559
130	TYR	CB	39.103
130	TYR	H	8.290
130	TYR	HA	4.561
130	TYR	N	122.002
131	GLU	C	173.707
131	GLU	CA	53.668
131	GLU	CB	30.124
131	GLU	H	8.318
131	GLU	HA	4.542
131	GLU	N	125.615
132	PRO	C	176.867
132	PRO	CA	62.947
132	PRO	CB	32.119
133	GLU	C	175.401
133	GLU	CA	56.462
133	GLU	CB	30.223
133	GLU	H	8.545
133	GLU	HA	4.211
133	GLU	N	121.670
134	ALA	C	172.574
134	ALA	CA	53.868
134	ALA	CB	20.047
134	ALA	H	8.020
134	ALA	HA	4.110
134	ALA	N	130.959